

tions to practical applications. Our work demonstrates the potential for seamlessly incorporating these advanced lithography methods into existing semiconductor fabrication workflows, thereby enhancing the overall capabilities of the industry.

Acknowledgments. This work was supported by project #2023.05/0022, funded by the National Research Foundation of Ukraine through a grant from the state budget.

COORDINATION COMPOUNDS WITH CHELATE LIGANDS IMMOBILISED ON NANOSILICA

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Ligands and coordination compounds immobilized on nanoparticle surfaces are widely used for extracting harmful metals and hazardous organic substances, as well as for creating drugs and precise catalysts. However, determining their structures, which dictate their properties, is challenging due to the lack of direct structural methods and the inaccuracy of indirect methods. Thus, quantum chemistry remains the most reliable approach for predicting the structure of immobilized complexes. On the example of vanadyl complexes with bidentate Schiff bases immobilized through an iminopropyl linker on the surface of silica, the possibilities of the formation of vanadyl complexes with the formation of bis and mono complexes were considered, and their structure was calculated using the restricted Hartree-Fock method for open shells (ROHF) with the SBKJC basis set. The structures of a few complexes with Schiff bases with various sterically hindered substituents were calculated, as well as the structures obtained with similar complexes with free ligands and crystal structures for single crystals of synthesized complexes of similar ligands from solution were compared. Vanadyl was chosen because the vanadium-oxygen double bond determines the axis of orientation in the complex structure.

The results demonstrate close parameters of the structures of the immobilized complexes, regardless of the steric complexity of the ligands (structures with different directions of vanadyl, oxygen to and from the surface were considered). However, the structure of immobilized complexes is significantly different from soluble analogues (see Fig.), which determine catalytic properties or bioactivity.

Thus, the steric hindrances of the ligands do not significantly affect the structure of the immobilized complexes, but the electronic donor-acceptor effect of the substituents on their properties will be decisive. However, the shape of the coor-

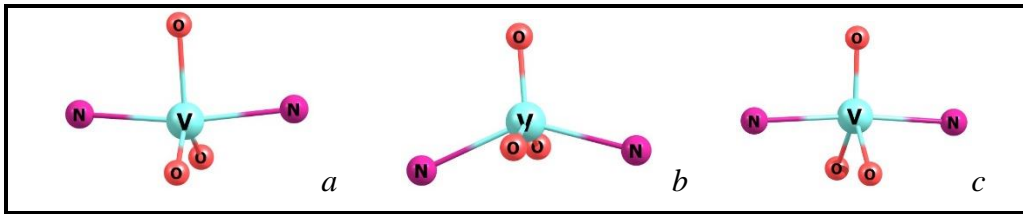


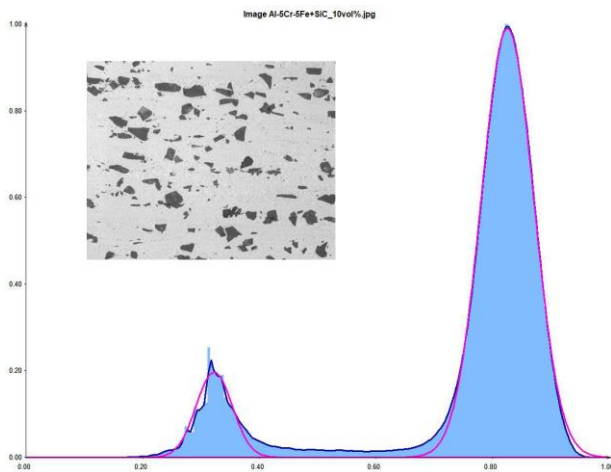
Fig. Coordination polyhedron of free (a) and immobilized salicylaldimines (b, c): (b) – V=O directed out of surface and (c) - V=O directed towards surface

dination polyhedron will be significantly influenced by the orientation of the vanadyl vector towards or away from the surface.

METHOD FOR QUANTITATIVE DETERMINATION OF THE COMPOSITION OF A TWO-PHASE NANOCOMPOSITE

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A new method for evaluation the quantitative analysis of the composition of two-component nanocomposite from an image is proposed. This method does not use a binarization threshold and has greater accuracy than traditional binarization methods.

Methods for evaluation the composition of a nanocomposite are based on the principle that the ratio of the area of one component to the area of another in a two-dimensional cross-sectional image of a three-dimensional object corresponds to the ratio of their volumes. The traditional solution to this problem is to determine a threshold brightness value, after which all pixels are divided into two groups based on their brightness relative to the threshold [1].

The proposed method is based on representing the brightness histogram as two normal distributions corresponding to two histogram peaks. The ratio of the areas under the Gaussian curves is used to obtain the quantitative value of the